

4,4'-(Propane-2,2-diyl)di(²H₄)phenol
92739-58-7 | DTXSID40662328

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 144 °C

Global applicability domain: Inside

Local applicability domain index: 9.10e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Bisphenol A</div> <div>Measured: 153</div> <div>Predicted: 144</div>	<div>Image not found</div> <div>4,4'-Propane-1,1-diylidiphenol</div> <div>Measured: 132</div> <div>Predicted: 133</div>	<div>Image not found</div> <div>phenol, 4,4'-butylidenebis-</div> <div>Measured: 137</div> <div>Predicted: 142</div>
<div>Image not found</div> <div>Bisphenol B</div> <div>Measured: 121</div> <div>Predicted: 140</div>	<div>Image not found</div> <div>meso-Hexestrol</div> <div>Measured: 187</div> <div>Predicted: 157</div>	